

# Optical Properties of Dopants and Impurities in III-Nitride Materials

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## Optical Properties of Dopants and Impurities in III-Nitride Materials

- The search for substitutional Si and Mg in GaN.  
Si-H and Mg-H complexes in GaN.
- Local vibrational modes of C-H complexes
- Intersubband transitions in GaN/AlGaN MQWs
- Sensors for detection of biological agents

# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Major issues associated with III-nitrides

### •Growth:

- $T_g = 750\text{ }^\circ\text{C}$  for MBE samples
- $T_g = 1050\text{ }^\circ\text{C}$  for MOCVD samples

### • Doping:

- Difficult to control the dopant incorporation
- As grown materials: GaN:  $V_N$ , n-type.

### •Substrates:

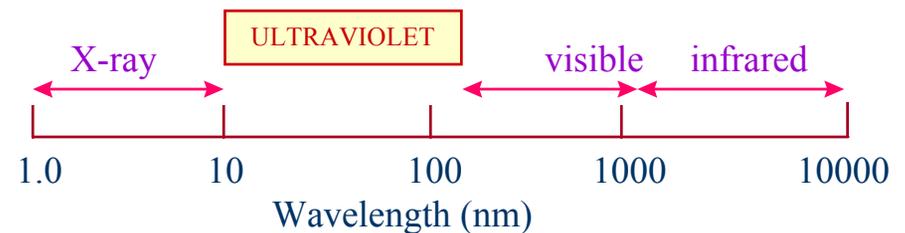
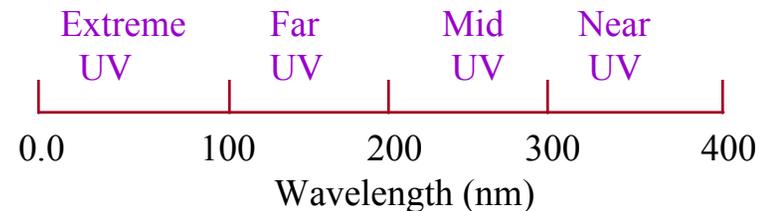
- $\text{Al}_2\text{O}_3$ , SiC, GaAs, Si
- stress due to lattice mismatch
- Misfit dislocations  $\sim 10^9\text{ cm}^{-3}$

### •Processing:

- Base-line processing is not well established
- Planar metallization
- Reactive ion etching is currently used in device fabrication

### •Related Compounds:

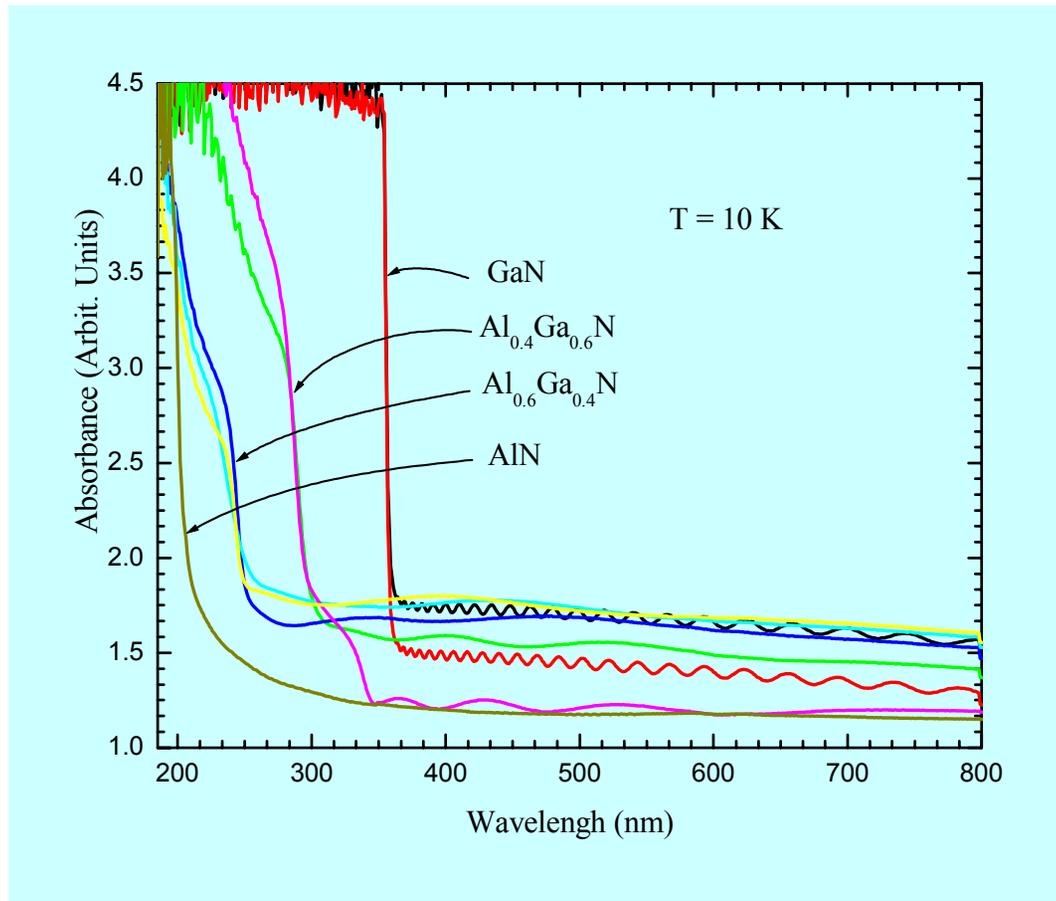
- $\text{In}_x\text{Ga}_{1-x}\text{N}$ : Difficult to incorporate In,  $x\sim 20\%$
- AlGaN: Much easier to grow.



Solar Blind = 100 – 300 nm  
Deep UV = 190 – 350 nm

# Optical Properties of Dopants and Impurities in III-Nitride Materials

Band edge absorption of AlGaN alloys showing the spectral range of UV detectors

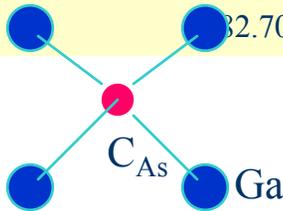


# Optical Properties of Dopants and Impurities in III-Nitride Materials

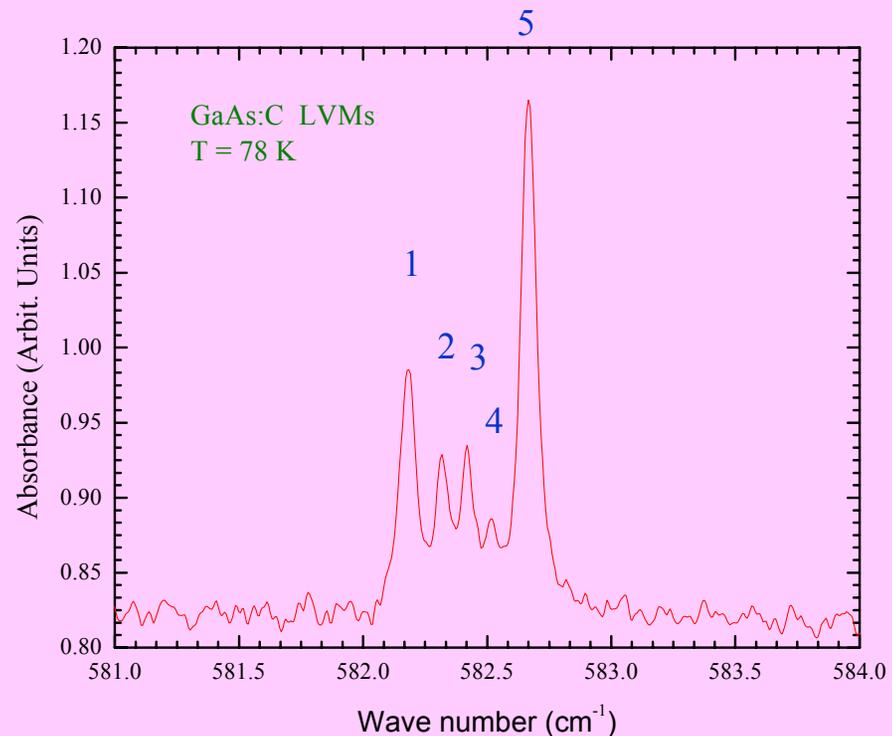
## Local Vibrational Modes of dopants and Impurities

Comparison of experimental and theoretical  $C_{As}$  LVMs in GaAs.

Symmetry	Experiment	Theory
$\bar{T}_d$ : Four $^{69}\text{Ga}$ atoms	582.95(5)	$F_2$ : 582.94
$T_d$ : Four $^{71}\text{Ga}$ atoms	582.46 (1)	$F_2$ : 582.46
$C_{2v}$ : two $^{71}\text{Ga}$ and two $^{69}\text{Ga}$ atoms	582.46 (1) 562.60 (2) 582.81(4)	$A_1$ : 582.44 $B_1$ : 582.61 $B_2$ : 582.80
$C_{3v}$ : three $^{71}\text{Ga}$ and one $^{69}\text{Ga}$ atoms	582.60 (2) 582.46 (1)	$A_1$ : 582.60 E: 582.45
$C_{3v}$ : one $^{71}\text{Ga}$ and three $^{69}\text{Ga}$ atoms	582.95 (5) 582.70 (3)	$A_1$ : 582.92 E: 582.70

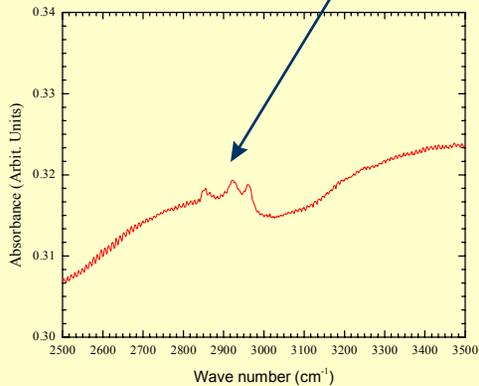


Doping: Example (Carbon in GaAs)

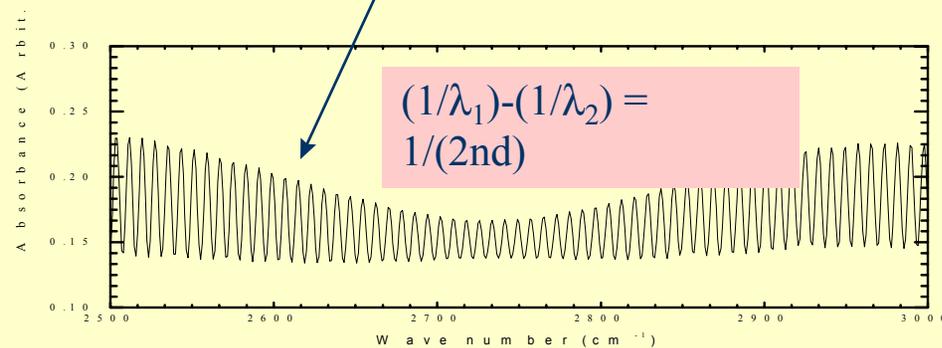
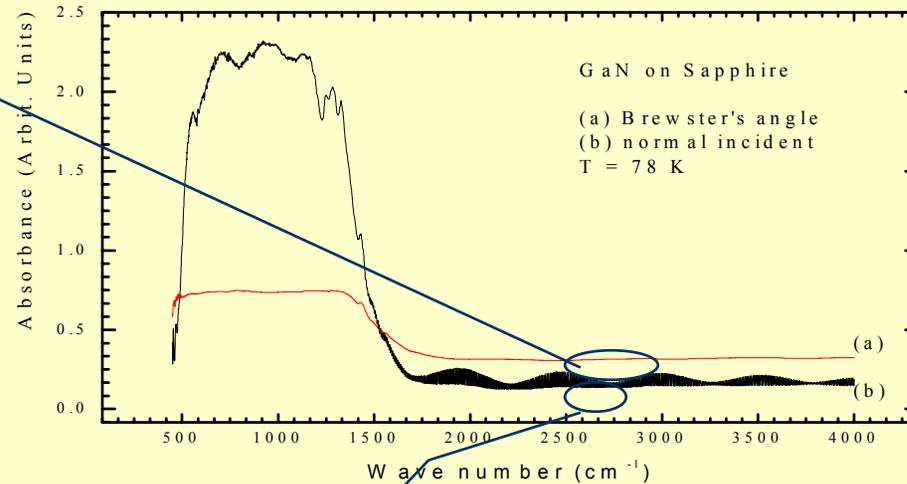


# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Local Vibrational Modes of dopants and Impurities



C-H LVMs



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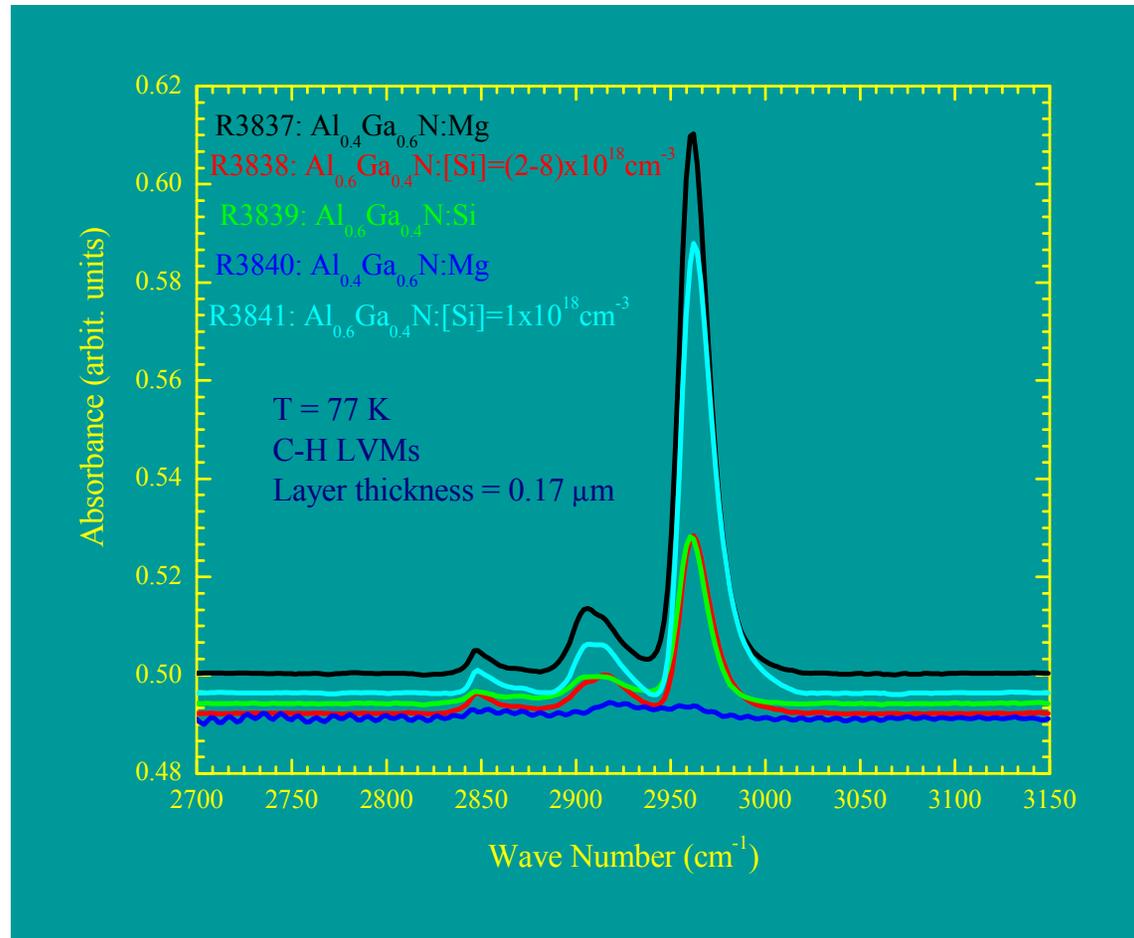
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## Local Vibrational Modes of dopants and Impurities

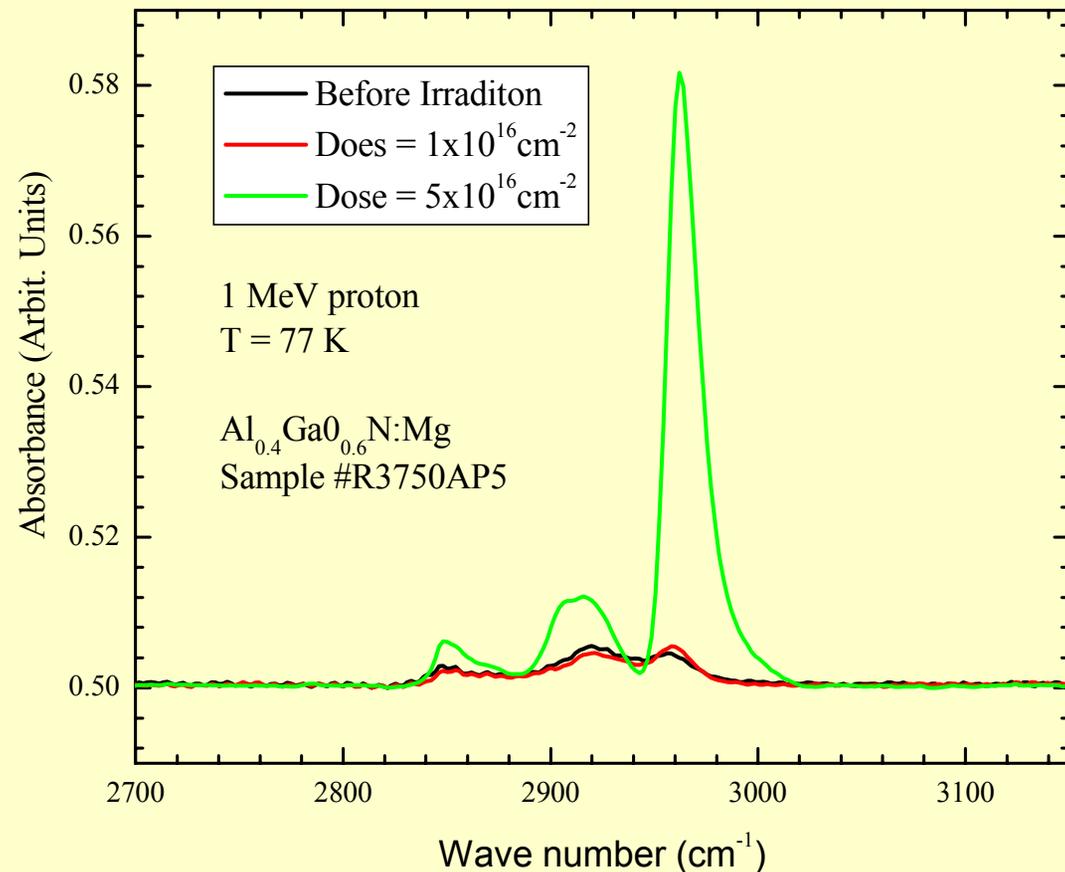
Local Vibrational modes  
of C-H<sub>n</sub> complex  
(n = 1, 2, or 3)



# Optical Properties of Dopants and Impurities in III-Nitride Materials

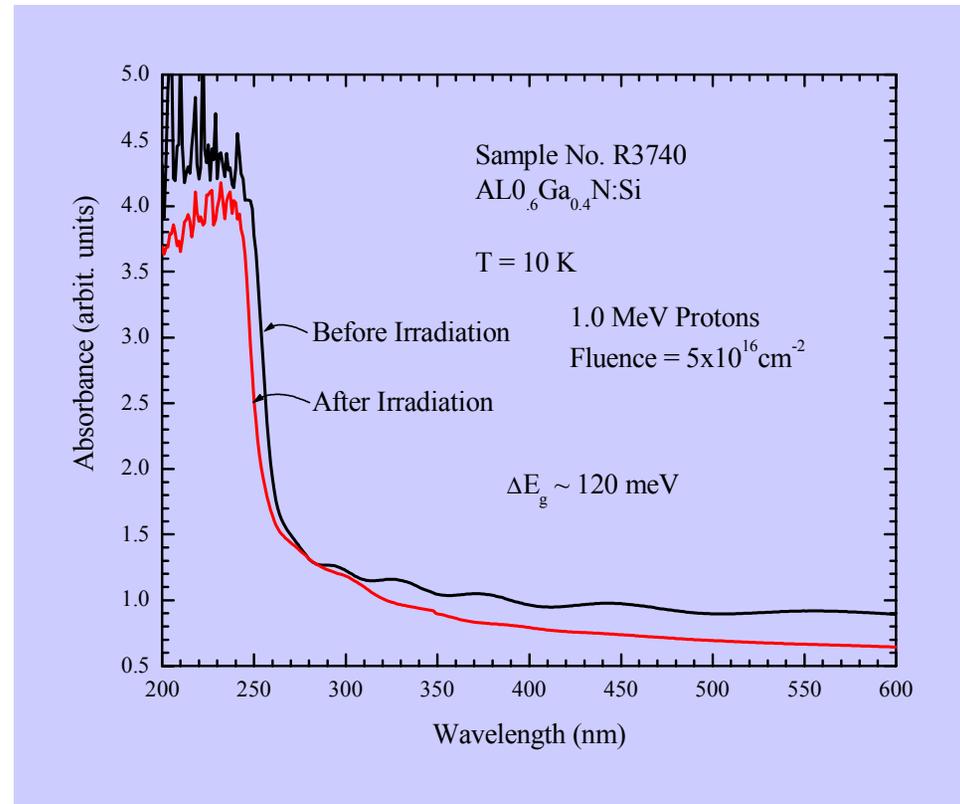
## Local Vibrational Modes of dopants and Impurities

Proton irradiation effect  
on C-H complexes.



# Optical Properties of Dopants and Impurities in III-Nitride Materials

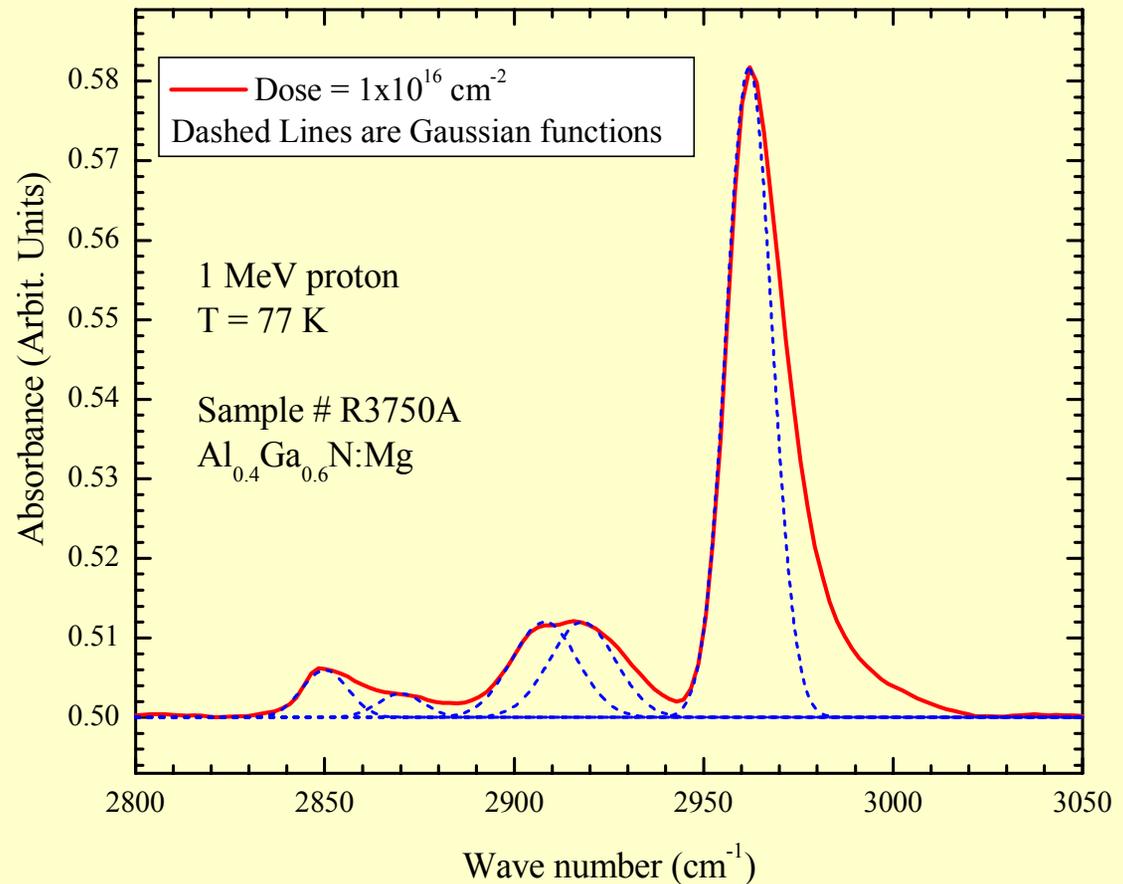
Proton irradiation effect on the band gap of AlGaN thin films grown on sapphire.



# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Local Vibrational Modes of dopants and Impurities

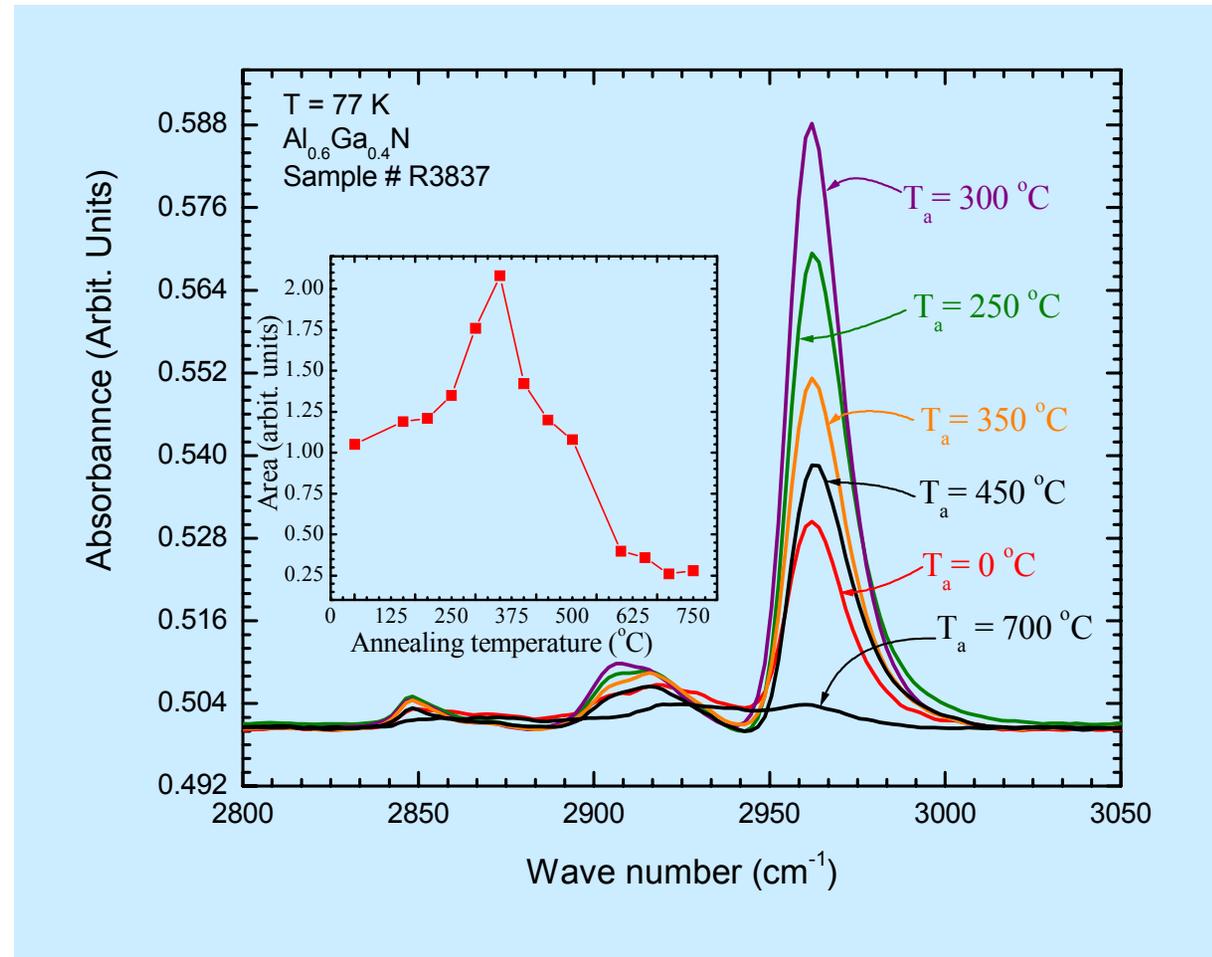
Peaks are related to symmetrical and asymmetrical stretching modes of C-H LVMs



# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Local Vibrational Modes of dopants and Impurities

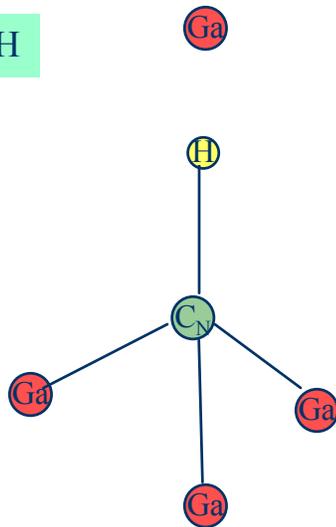
Thermal annealing effect on the C-H LVMs in AlGaN



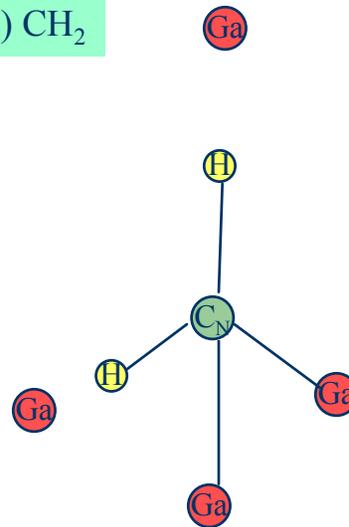
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## Local Vibrational Modes of dopants and Impurities

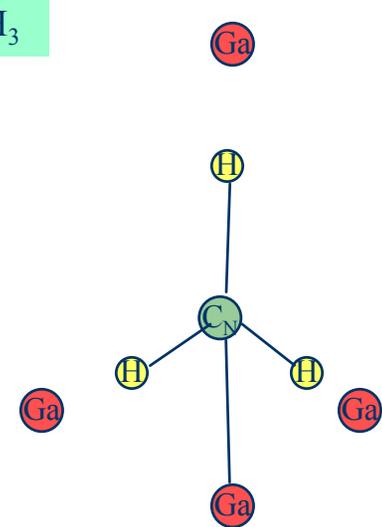
(a) CH



(b) CH<sub>2</sub>



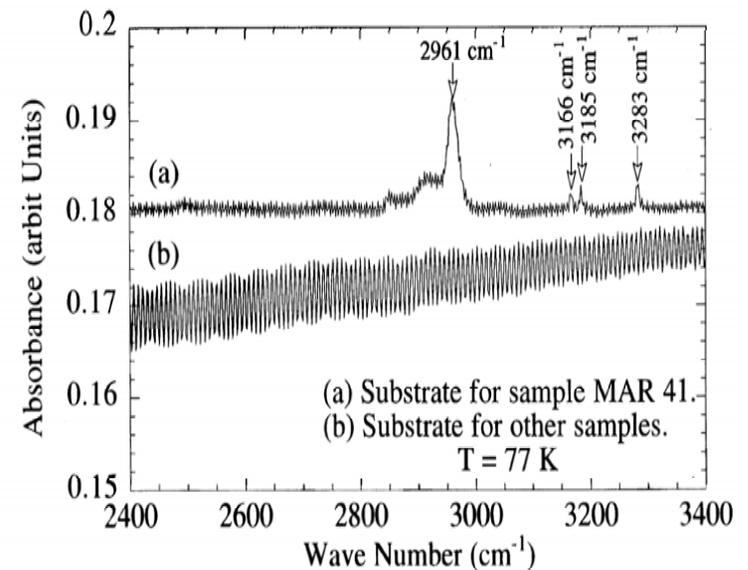
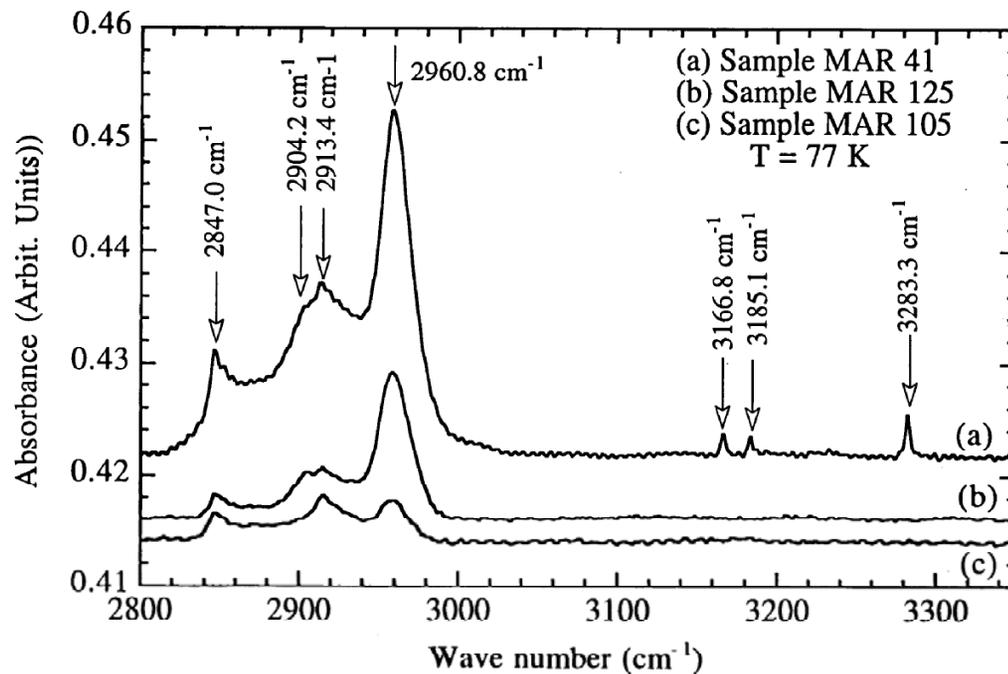
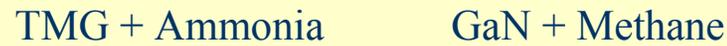
(c) CH<sub>3</sub>



Group	Stretching Modes	Observed (cm <sup>-1</sup> )	Calculated (cm <sup>-1</sup> )
CH		2851.7	2850.0
CH <sub>2</sub>	Asymmetric	2911.9	2949.0
CH <sub>2</sub>	Symmetric	2918.0	2902.0
CH <sub>3</sub>	Asymmetric	2962.0	2950.0
CH <sub>3</sub>	Symmetric	2872.0	2878.0

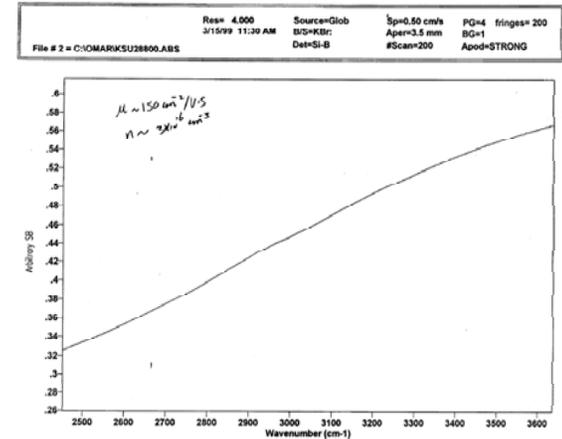
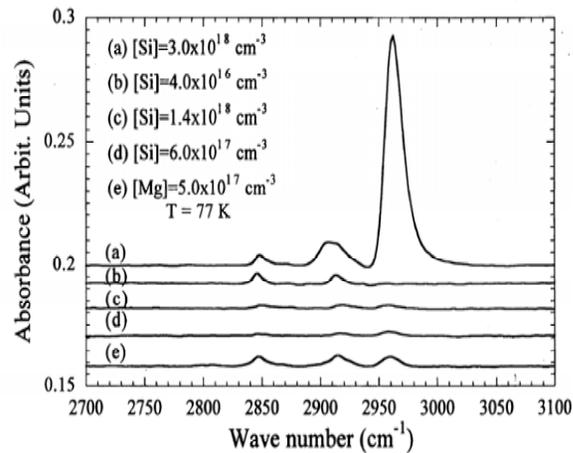
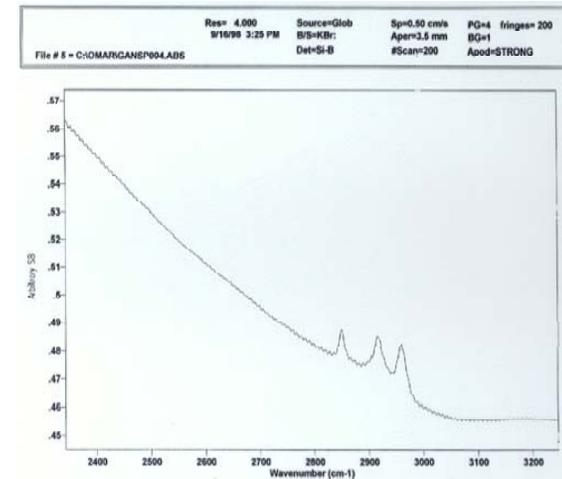
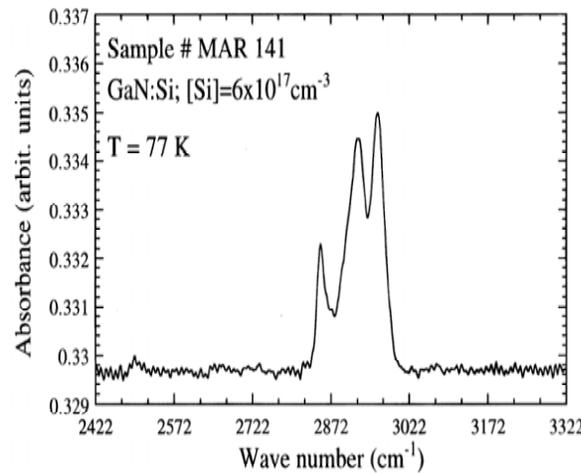
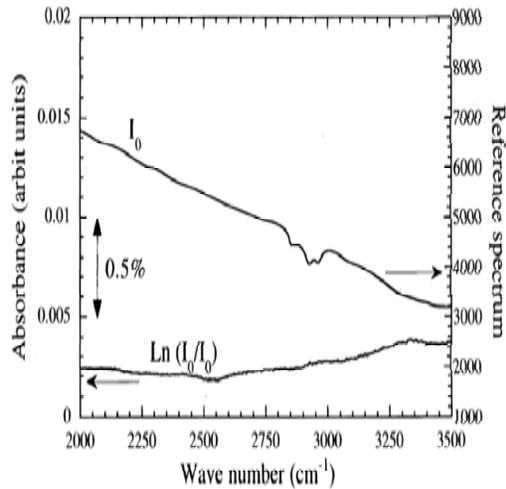
# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Local Vibrational Modes of dopants and Impurities



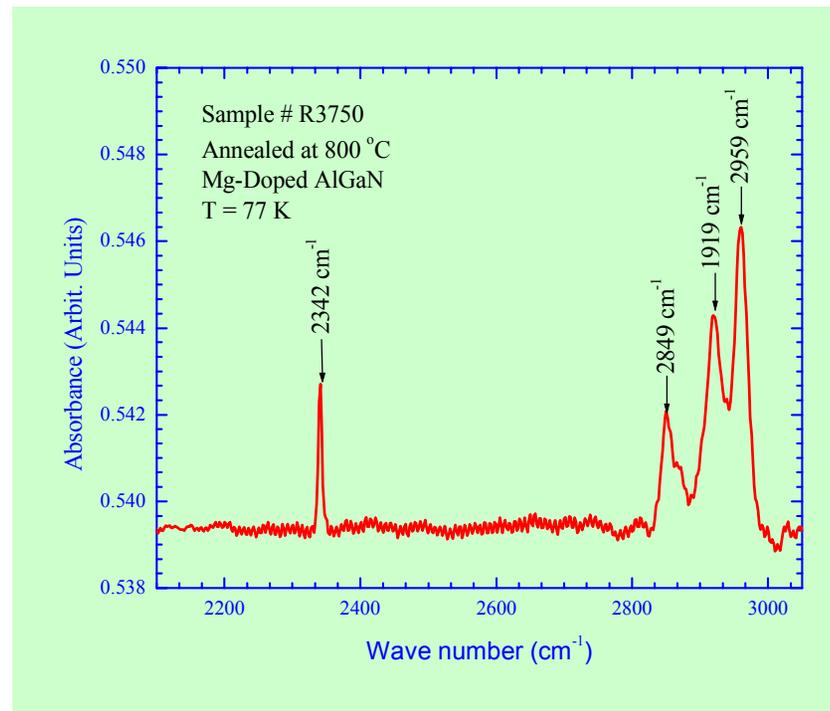
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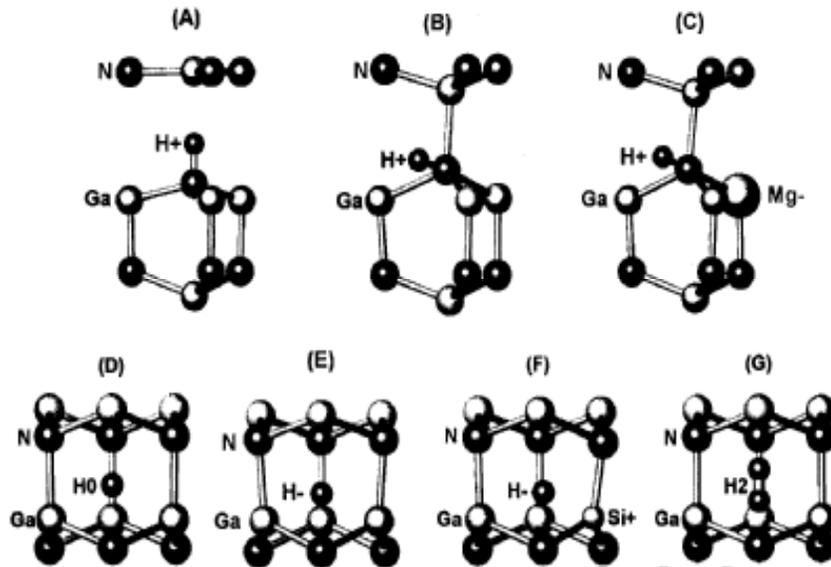
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## Equilibrium state of hydrogen in gallium nitride: Theory and experiment

S. M. Myers,<sup>a)</sup> A. F. Wright, G. A. Petersen, C. H. Seager, W. R. Wampler,  
M. H. Crawford, and J. Han  
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## Local Vibrational Modes of dopants and Impurities

FIG. 1. Minimum-energy configurations of H in wurtzite GaN obtained from density-functional theory. The projection is orthographic, allowing lattice relaxations to be discerned. The energy of H<sup>+</sup> does not differ significantly between the configurations in (a) and (b).

TABLE I. Properties of H in GaN at zero temperature from density-functional theory. The formation-energy reference state comprises the neutral H atom in vacuum and GaN with electronic dopants neutral. Vibrational frequencies are divided by the speed of light, *c*.

Species	Formation energy at $E_F = E_g$ (eV/H atom)	Diffusion activation energy <sup>a</sup> (eV)	Vibration frequency/ <i>c</i> (cm <sup>-1</sup> )
H <sup>0</sup>	+0.34	0.6	692 (c axis) 816 (l. c axis, two modes)
H <sup>+</sup> (AB) <sup>b</sup>	-2.67	0.7	2970 (N-H stretch) 847 (bend, two modes)
H <sup>+</sup> (BC) <sup>c</sup>	-2.67	0.7	3420 (N-H stretch) 502 (bend, two modes)
H <sup>-</sup>	+1.52	1.6	1216 (c axis) 1406 (l. c axis, two modes)
H <sub>2</sub>	-1.40		4235 (mol. stretch) 1091 (displ. c axis) 1384 (displ. l. c axis, two modes) 1012 (shear l. c axis, two modes)
	Binding energy <sup>d</sup> (eV)		
MgH	-0.7		3284 (N-H stretch) 937 (bend, two modes)
SiH	-0.3		1739 (Si-H stretch) 1302, 1427 (bend)

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# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Intersubband transitions in MQWs

Structure:

GaAs/AlGaAs MQWs

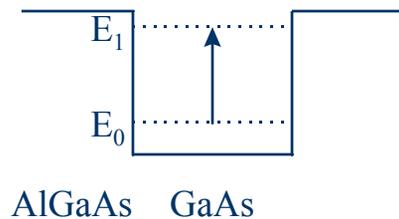
well: 75 Å Si doped  $\{[Si] \sim 2 \times 10^{18} \text{ cm}^{-3}\}$

barrier: 100 Å, Al-mole fraction=30%

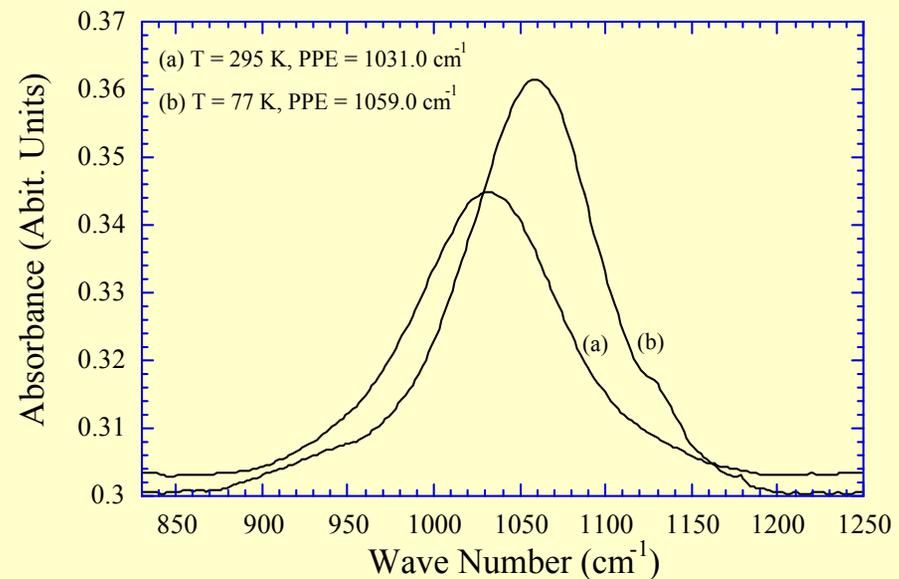
50 periods

Temperature blueshift

PPE blueshifts with decrease in temperature on average  $\sim 30 - 50 \text{ cm}^{-1}$



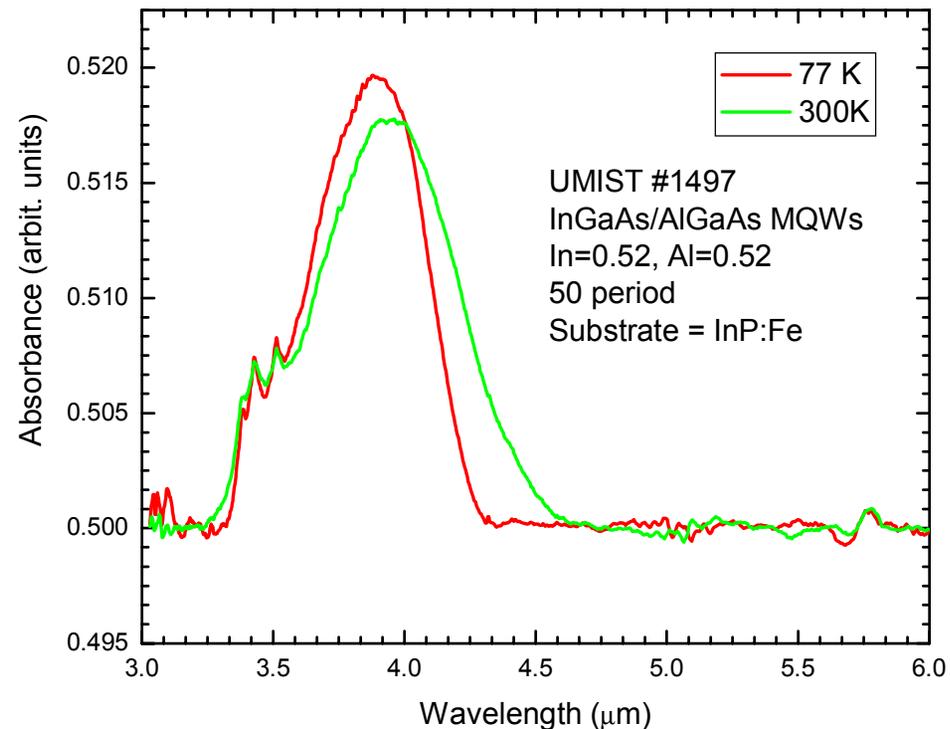
Long wavelength infrared applications



# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Intersubband transitions in MQWs

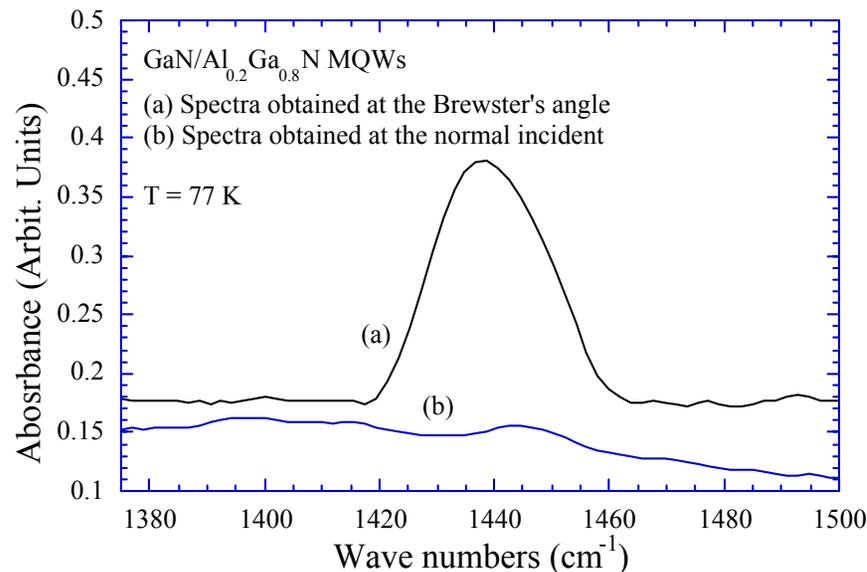
Intersubband transition in InGaAs/InAlAs MQWs. In=0.52, Al=0.52, period = 50, the well is doped with [Si]= $6 \times 10^{18} \text{cm}^{-3}$ , the substrate is InP:Fe, and the cap layer is 50Å InGaAs:Si. The well width= 30Å and the barrier width = 300Å.



# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Intersubband transitions in GaN/AlGaN MQWs

Intersubband transition in GaN/Al<sub>0.2</sub>Ga<sub>0.8</sub>N multiple quantum wells spectra measured at the Brewster's angle (a) and at the normal incident (b). The total number of the multiple quantum wells is 30. The well thickness is 30Å and the barrier thickness is 100Å.



# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Intersubband transitions in GaN/AlGaN MQWs

Appl. Phys. Lett., Vol. 77, No. 23, 4 December 2000

Gmachl et al,

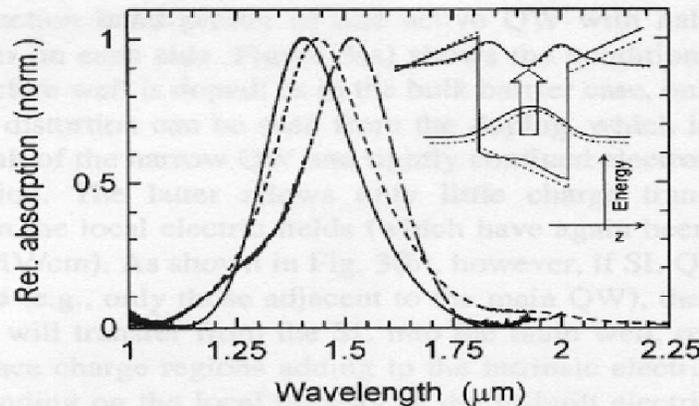


FIG. 1. Normalized intersubband absorption spectra of three samples containing 11 (dashed), 12 (solid), and 13 (dashed-dotted) Å wide GaN MQWs. The barrier material is  $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ ; and the structures were grown on an  $\text{Al}_{0.65}\text{Ga}_{0.35}\text{N}$  buffer layer. *Inset*: Conduction band profile and moduli squared of the electron wave functions of a 13 Å wide GaN QW calculated by self-consistently solving Poisson's and Schroedinger's equation for a doping level in the well of  $1 \times 10^{20} \text{ cm}^{-3}$  (solid) and for an undoped (dashed) QW. The open arrow indicates the absorption process.

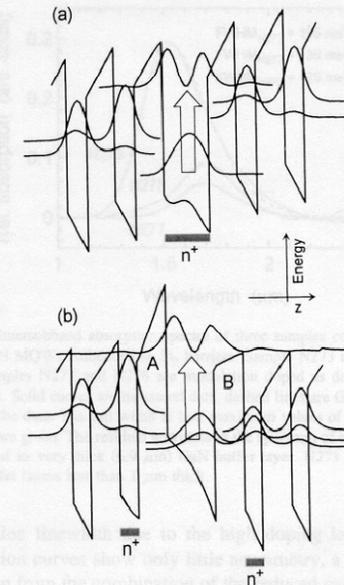
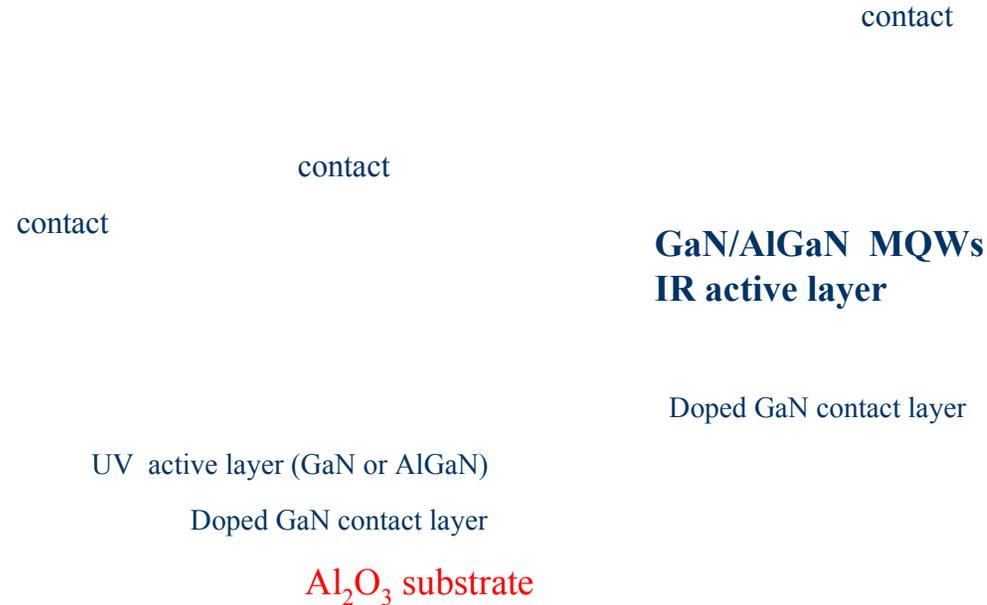


FIG. 3. Conduction band profiles and moduli squared of the electron wave functions calculated for a 16 Å wide GaN QW with SL barriers by self-consistently solving Poisson's and Schroedinger's equation for a doping level of  $\sim 1 \times 10^{20} \text{ cm}^{-3}$ . The superlattices consisted of 10 Å wide  $\text{Al}_{0.65}\text{Ga}_{0.35}\text{N}$  barriers and 6–7 Å wide GaN wells. The gray bars indicate the location of the dopant atoms. The open arrow indicates the absorption process; (a) shows the case of a well doped structure. (b) shows a modulation doped structure. "A" and "B" in (b) indicate SL barriers in which the electric field is enhanced and decreased, respectively, by the space charge induced by electron transfer from the SL regions into the main QW. "z" indicates the growth direction.

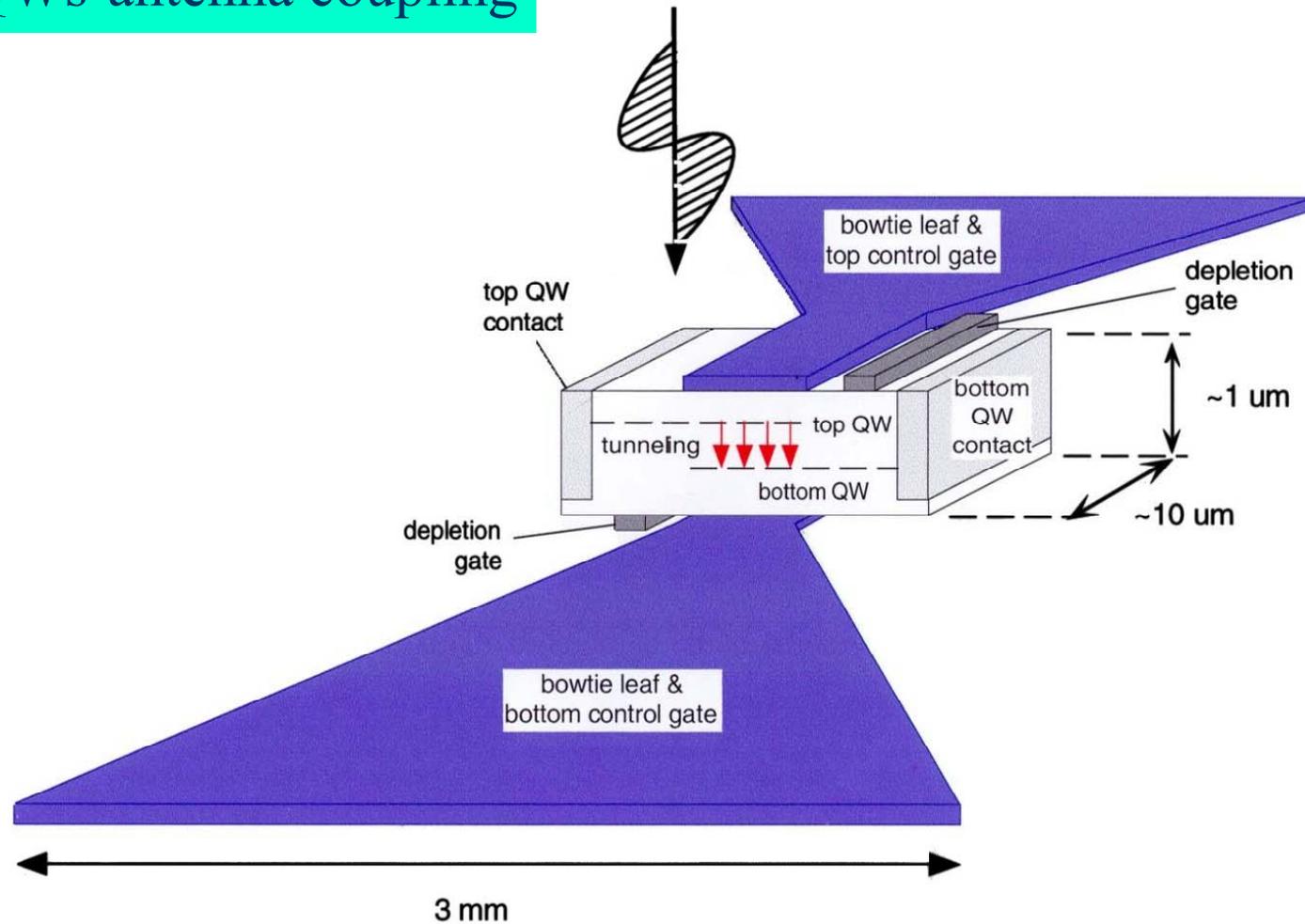
# Optical Properties of Dopants and Impurities in III-Nitride Materials



A possible scheme of the proposed UV-IR detector. The UV detection region is based on the interband transitions in GaN and or AlGaN epitaxial layer. The IR detection region is based on the intersubband transitions in GaN/AlGaN and/or GaN/AlN multiple quantum wells (MQWs).

# Optical Properties of Dopants and Impurities in III-Nitride Materials

## MQWs-antenna coupling



# Optical Properties of Dopants and Impurities in III-Nitride Materials

## Antigen detections

